Letters to the Editor

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Debye characteristic temperature of ionic crystals

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In this note we have calculated the effects of lattice anharmonicity only due to thermal expansion, on the Debye characteristic temperature of KBr, KCl and NaF, in the high temperature range using the formulation of Willis (1969) and the usual Debye-Waller formula. The Debye-Waller formula represents the temperature factor of cubic crystals of simple type with fair accuracy, so long as the temperature is not high. At high temperatures, however, the increasing expansion of the crystal causes change in its elastic properties and the assumption of a constant characteristic temperature in the formula for M (exponent of the Debye-Waller factor e^{-2M}) is no longer justifiable At higher temperatures, therefore, the simple theory breaks down. Willis has given a formula for estimating the change of B-factor and thereby Θ with temperature.

In the classical limit of temperature, Debye characteristic temperature is given by

$$\frac{1}{\Theta^2} = \frac{mk_B^2}{3\hbar^2\alpha_0}\left[1+T\left(2\chi\gamma_G-20K_B\frac{\gamma_0}{\alpha_0^2}\right)\right] \qquad (1)$$

where α_0 is the harmonic parameter defined by

$$\alpha_0 = 8\pi^2 k_B T/B^h(T),$$

γ_G, the Gruneisen parameter and χ the volume expansion coefficient.

The experimental Debye characteristic temperatures of KBr, KCl and NaF have been taken from Pathak & Trivedi (1971) determined by X-ray diffraction upto about 800°K. Comparison of the experimental results with present calculated values is shown in figure 1 as plots of Θ *vs* T for KBr, KCl and NaF. The dotted line corresponds to the harmonic theory based on Buyers & Smith's (1968) calculations. Because of the effect of anharmonicity, the experimental points lie appreciably below this line at higher temperatures. The solid line is drawn using eqn. (1) in its quasi-harmonic form, that is by retaining the thermal expansion term but taking $\gamma_0/\alpha_0^2 = 0$. In calculations, Grüneisen constants were taken from Born & Huang (1954) and volume expansion coefficients from Weyl (1955).

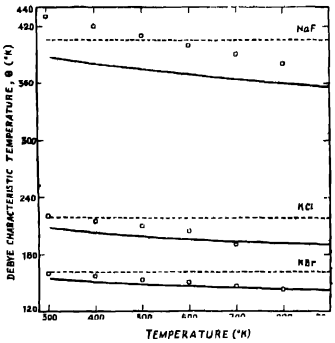

Figure 1. Calculated and experimental values of Debye characteristic temperature Θ, plotted against temperature T. Dotted line : harmonic calculations of Buyers & Smith (1968); Solid line : quasi-harmonic perturbation theory results.

Comparing the theoretical curves with experiment we see that except for NaF upto 400°K, the harmonic theory agrees well with the experimental results. Above this temperature the anharmonic vibrations become increasingly important and so a better agreement is obtained using the quasi-harmonic theory. The existing discrepancy between theory and experiment is due to the neglect of the additional anharmonic corrections (not necessarily of the same sign) that occur even when the crystal is held at constant volume (Maradudin & Flinn 1963) and due to lack of good analysis of the experimental data.

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